X-17404

UNCLASSIFIED

CF-54-8-97

Subject Category: PHYSICS

UNITED STATES ATOMIC ENERGY COMMISSION

CALCULATION OF FISSION NEUTRON AGE IN $NaZrF_5$

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Technical Information Service, Oak Ridge, Tennessee

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Date Declassified: December 16, 1955.

~~Printed in USA, Price 15 cents. Available from the Office of Technical Services, Department of Commerce, Washington 25, D. C.~~

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Work performed under Contract No. W-7405-Eng-26.

OAK RIDGE NATIONAL LABORATORY
Operated By
CARBIDE AND CARBON CHEMICALS COMPANY
POST OFFICE BOX P
OAK RIDGE, TENNESSEE

Calculation of Fission Neutron Age in $NaZrF_5$

One of the limits imposed on experimental measurements of the neutron age of various materials is the size required for the experimental setup if the age is too great. In the case of $NaZrF_5$, a calculation has been made to determine if this is a limiting factor in the measurement of age to indium resonance.* In the calculation it is assumed that it is possible to apply the Fermi age theory for the distribution of neutrons.

<u>Method of Calculation</u>

For a monoenergetic point source of neutrons, the solution of the age equation is[1]

$$q(r,\tau) = \frac{Q}{(4\pi\tau)^{3/2}} \, e^{-r^2/4\tau} \tag{1}$$

where

r = distance from point source,

Q = number of neutrons emitted per second by the source,

q = neutron slowing down density.

The age τ is defined[1] by

$$\tau(E_o,E) = \int_E^{E_o} \frac{\lambda^2(E')\, dE'/E'}{3\,\xi(1 - \overline{\cos\theta})} \tag{2}$$

where

E = neutron energy,

E_o = source energy,

$\lambda(E)$ = mean free path at energy E,

ξ = average loss in logarithm of energy upon collision,

$\overline{\cos\theta}$ = average cosine of angle between neutron direction before and after collision in laboratory system.

* The age to indium resonance is the square of what is usually called the "slowing down length" to indium resonance.

1 Jay Orear, A. H. Rosenfeld, and R. A. Schluter, <u>Nuclear Physics</u>, University of Chicago Press, Chicago, 1950.

The mean square slowing down length, $\overline{R^2}$, is given by

$$\overline{R^2} = \frac{\int_0^\infty r^2\, q(r,\tau)dV}{\int_0^\infty q(r,\tau)dV} \tag{3}$$

$$= \frac{\int_0^\infty r^2 \frac{Q}{(4\pi\tau)^{3/2}}\, e^{-r^2/4\tau}\, 4\pi r^2 dr}{\int_0^\infty \frac{Q}{(4\pi\tau)^{3/2}}\, e^{-r^2/4\tau}\, 4\pi r^2 dr} \tag{3a}$$

In the case in which the source is not monoenergetic, its energy distribution being described by f(E),

$$q(r,E) = \int_E^\infty dE'f(E')\, \frac{Q\, e^{-r^2/4\left[\tau(E',E'')-\tau(E,E'')\right]}}{\left\{4\pi\left[\tau(E',E'') - \tau(E,E'')\right]\right\}^{3/2}} \tag{4}$$

where E" is some lower energy. If $\overline{R^2}(E)$ is computed from Eqs. (3) and (4) it is found that

$$\frac{\overline{R^2}(E)}{6} = \int_E^\infty f(E')dE'\tau(E',E) \tag{5}$$

The right-hand expression of Eq. (5) will be called the <u>age to energy E</u> for the distribution f(E). Integrating by parts,

$$\int_E^\infty f(E')dE'\,\tau(E',E) = -\,\tau(E',E)\int_{E'}^\infty f(E'')dE''\,\Bigg|_{E'=E}^{\infty} +$$

$$\int_E^\infty dE'\,\frac{d}{dE'}\,\tau(E',E)\int_{E'}^\infty f(E'')dE'' \tag{6}$$

It is reasonable to assume that the first term on the right-hand side of Eq. (6) vanishes. Thus

$$\tau(E) = \int_E^\infty dE'\,\frac{d\tau}{dE'}\,(E',E)\int_{E'}^\infty f(E'')dE'' \tag{7}$$

where $\tau(E)$ is the age to energy E for the distribution f(E). If the value of $d\tau/dE$ is derived from Eq. (2) and substituted in Eq. (7),

$$\int_E^\infty \frac{\lambda^2(E')dE'}{3\xi E'(1-\overline{\cos\theta})}\int_{E'}^\infty f(E'')dE'' = \tau(E) \tag{8}$$

For the case of a fission spectrum

$$f(E) = \sqrt{\frac{2}{\pi e}}\; e^{-E}\sinh\sqrt{2E}$$

where E is the neutron energy (Mev). It is easier for the purposes of integration to change variables by the transformation $E = V^2/2$. Thus

$$f(E)dE = \left[\sqrt{\frac{2}{\pi e}}\; e^{-V^2/2}\sinh V\right] VdV \tag{9}$$

$$\sqrt{\frac{2}{\pi e}}\, V dV e^{-V^2/2} \sinh V \equiv \sqrt{\frac{2}{\pi e}}\, \frac{e^{1/2}}{2}\Big[(V-1)dVe^{-(V-1)^2/2} + dVe^{-(V-1)^2/2} - (V+1)dVe^{-(V+1)^2/2} + dVe^{-(V+1)^2/2}\Big] \qquad (10)$$

$$\int_E^\infty f(E')dE' = \int_{V(E)}^\infty \frac{dV'}{\sqrt{2\pi}}\Big[(V'-1)e^{-(V'-1)^2/2} + e^{-(V'-1)^2/2} - (V'+1)e^{-(V'+1)^2/2} + e^{-(V'+1)^2/2}\Big]$$

$$= \frac{G(V)}{\sqrt{2\pi}} \qquad (11)$$

where

$$G(V) = e^{-(V-1)^2/2}\Big[1 - F(1-V)\Big] - e^{-(V+1)^2/2}\Big[1 - F(V+1)\Big] + \sqrt{2\pi} \qquad \text{for } V \leq 1$$

$$= e^{-(1/2)(V-1)^2}\Big[1 + F(V-1)\Big] - e^{-(V+1)^2/2}\Big[1 - F(V+1)\Big] \qquad \text{for } V \geq 1 \qquad (12)$$

$$F(x) = e^{x^2/2}\int_x^\infty e^{-t^2/2}\,dt \qquad \text{(see ref. 2)} \qquad (13)$$

Clearly $G(0) = \sqrt{2\pi}$. Substituting in Eq. (8),

$$\tau(E) = \int_{V(E)}^\infty \frac{dV'(2\lambda^2/V')\,G(V')}{3\,\xi(1 - \overline{\cos\theta})\sqrt{2\pi}} \qquad (14)$$

2 W. F. Sheppard, "The Probability Integral," Brit. Assoc. Advance. Sci, Math. Tables, Vol. VII, University Press, Cambridge, 1939.

The advantage of Eq. (14) is that $G(V)$ may be expressed analytically while the other terms may be directly computed from the cross sections. Thus with Eq. (14) it would only be necessary to do one numerical integration. With Eq. (5) it would be necessary to first compute $\tau(E',E)$ by numerical integration and then perform a second numerical integration to obtain $\tau(E)$. On the other hand, it is sometimes true that $\tau(E',E)$ is available from experimental data, in which case it would be advantageous to use Eq. (5).

Numerical Results

Values of $G(V)$ that were computed are given in Table 1. To aid in the integration, polynomial fits were made to $G(V)$.

$$G(V) = 2.5066 + 0.1392V - 0.4708V^2 \qquad \text{for } 0 \leq V \leq 1, \quad 0 \leq E \leq 0.5 \tag{15}$$

$$G(V) = 3.3535 - 1.1785V \qquad \text{for } 1 \leq V \leq 2, \quad 0.5 \leq E \leq 2 \tag{16}$$

$$G(V) = 2.6053 - 0.8044V \qquad \text{for } 2 \leq V \leq 3, \quad 2 \leq E \leq 4.5 \tag{17}$$

$$G(V) = 0.7249 - 0.1776V \qquad \text{for } 3 \leq V \leq 4, \quad 4.5 \leq E \leq 8 \tag{18}$$

$$G(V) = 0.0709 - 0.0141V \qquad \text{for } 4 \leq V \leq 5, \quad 8 \leq E \leq 12.5 \tag{19}$$

Equations (15) through (19) give polynomial fits to $G(V)$ for the ranges of V indicated. The corresponding values of the energy in Mev are also indicated. The error in the quadratic fit is about 1%. The maximum error in Eq. (16) is about 10%. In the remainder of the linear fits, the maximum percentage errors

Table 1

Values of G(V)

V	G(V)	V	G(V)
0.0	2.5066	1.0	2.1750
0.1	2.5062	1.5	1.4328
0.2	2.5034	2.0	0.9965
0.3	2.4959	2.5	0.4905
0.4	2.4815	3.0	0.1921
0.5	2.4585	3.5	0.0595
0.6	2.4253	4.0	0.0145
0.7	2.3808	4.5	0.0028
0.8	2.3243	5.0	0.0004
0.9	2.2556		

become steadily worse, but the absolute error is about the same. Furthermore, in the integration, $G(V)$ is weighted by a factor of $1/V$ so that the lower values of V are more important. The value of E_0 that will be used is 1.44 ev, the indium resonance energy. The corresponding value of V is 1.697 x 10^{-3}. Strictly, the normalizing factor in Eq. (14) should be $G\left[V(E_0)\right]$ instead of $\sqrt{2\pi}$, but since E_0 is so low no appreciable error is introduced.

To evaluate Eq. (14) with the polynomial fits, another approximation was made. By the theorem of mean value

$$\int_{V_1}^{V_2} \frac{dV(2\lambda^2/V)G(V)}{3\xi(1-\overline{\cos\theta})\sqrt{2\pi}} = \overline{\left[\frac{2\lambda^2}{3\xi(1-\overline{\cos\theta})\sqrt{2\pi}}\right]} \int_{V_1}^{V_2} \frac{G(V)}{V}\,dV \qquad (20)$$

where the bar over the expression in brackets denotes some value between V_1 and V_2. If the polynomial fits are used, the integral on the right-hand side of Eq. (20) may be evaluated exactly. It is then possible to obtain upper and lower limits for the integral on the left-hand side by using upper and lower limits for the expression in brackets.

To test the accuracy of this method, the age in graphite (density = 1.6 g/cc) was calculated. The quantities ξ and $\overline{\cos\theta}$ are constant. Table 2 gives the maximum and minimum values of the quantity $\int \frac{G(V)\lambda^2 dV}{V}$ from which the age for graphite can be determined:

$$(1.31)\left(\frac{2}{\sqrt{2\pi}}\right)\left(\frac{A}{\rho N_0 \times 10^{-24}}\right)^2\left(\frac{1}{3\xi(1-\overline{\cos\theta})}\right) = 362 \text{ cm}^2 \text{ (max.)}$$

$$(0.94)\left(\frac{2}{\sqrt{2\pi}}\right)\left(\frac{A}{\rho N_0 \times 10^{-24}}\right)^2\left(\frac{1}{3\xi(1-\overline{\cos\theta})}\right) = 260 \text{ cm}^2 \text{ (min.)}$$

where

A = atomic weight of carbon,

Table 2

Maximum and Minimum Values of
$\int \frac{G(V)\lambda^2 dV}{V}$ for Graphite

E(Mev)	$\int \frac{G(V)dV}{V}$	$\lambda^2 \times 10^2$ (barn^{-2}) Max.	Min.
1.44×10^{-6} - .08	13.710	4.73	4.73
0.08 - 0.5	1.947	8.5	4.73
0.5 - 2	1.146	34.6	8.5
2 - ∞	0.285	34.6	34.6
Sum of $\int \frac{G(V)dV}{V} \times \lambda^2$		1.31	0.94

ρ = density of carbon = 1.6 g/cc,

N_o = Avogadro's number.

The average between the upper and lower limits gives an age of 311 cm^2 for carbon which differs by only 6% from the experimental value[3] of 330 cm^2.

Application of Method to $NaZrF_5$

In an application of this method to the compound $NaZrF_5$ the density was taken as 4 g/cc,[4] and the quantities ξ and $\overline{\cos\theta}$ were taken as the average of the quantities for Na, Zr, and F weighted by the cross sections and the relative amount of each element in the compound. Table 3 gives the maximum value of the quantity $x^2/3\,\xi(1 - \overline{\cos\theta})$ for the energy range listed; Table 4 gives the minimum value for the same quantity. In these calculations $12.5 = \infty$. From Table 3 the upper estimate on the age may be obtained by

$$(89.372 \times 10^{-3}) \left(\frac{2}{\sqrt{2\pi}}\right)\left(\frac{A}{\rho N_o \times 10^{-24}}\right)^2 = 538 \text{ cm}^2$$

where

A = molecular weight of $NaZrF_5$,

ρ = density of $NaZrF_5$ = 4 g/cc,

N_o = Avogadro's number.

Similarly, the lower limit is estimated from Table 4 as 328 cm^2. The average between the upper and lower limits is 433 cm^2 which gives an estimate of the age in $NaZrF_5$ as

$$\tau(1.44 \text{ ev}) = 433 \pm 105 \text{ cm}^2 = 433\ (1 \pm 0.25) \text{ cm}^2 \qquad (21)$$

The number 105 is the difference between the mean and either the upper or lower estimates.

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3 J. E. Hill, L. D. Roberts, and G. E. McCammon, "Slowing Down of Fission Neutrons in Graphite," ORNL-187 (Jan. 19, 1949).

4 W. K. Ergen, personal communication.

Table 3

Maximum Value of $\int \frac{G(V)\lambda^2 dV}{3\xi(1 - \overline{\cos\theta})V}$ for $NaZrF_5$

E(Mev)	$\lambda^2/3\xi(1 - \overline{\cos\theta}) \times 10^3$ (barn^{-2})	$\int_{V_1}^{V_2} \frac{G(V)}{V} dV$
1.44×10^{-6} to 2×10^{-3}	5.5	9.0770
2×10^{-3} to 2.5×10^{-3}	2.8	0.2803
2.5×10^{-3} to 3×10^{-3}	0.9	0.2293
3×10^{-3} to 4×10^{-3}	2.5	0.3616
4×10^{-3} to 6×10^{-3}	3.0	0.5099
6×10^{-3} to 2.5×10^{-2}	4.4	1.7957
2.5×10^{-2} to 1.0×10^{-1}	3.3	1.7334
1.0×10^{-1} to 1.1×10^{-1}	0.5	0.1176
1.1×10^{-1} to 2.5×10^{-1}	3.5	0.9962
2.5×10^{-1} to 3.5×10^{-1}	1.7	0.3928
3.5×10^{-1} to 5×10^{-1}	2.4	0.3390
5×10^{-1} to 2.0	13.0	1.1460
2 to ∞	8.2	0.2846
Sum of $\left[\lambda^2/3\xi(1 - \overline{\cos\theta}) \times 10^3\right]$	$\left[\int_{V_1}^{V_2} \frac{G(V)}{V} dV\right]$	89.372

Table 4

Minimum Value of $\int \frac{G(V)\lambda^2 dV}{3\xi(1 - \overline{\cos\theta})V}$

for $NaZrF_5$

E(Mev)	$\lambda^2/3\xi(1 - \overline{\cos\theta}) \times 10^3$ (barn^{-2})	$\int_{V_1}^{V_2} \frac{G(V)}{V} dV$
1.44×10^{-6} to 1.6×10^{-3}	4	8.7965
1.6×10^{-3} to 2.2×10^{-3}	1.8	0.4001
2.2×10^{-3} to 4×10^{-3}	0.78	0.7487
4×10^{-3} to 6×10^{-3}	1.6	0.5099
6×10^{-3} to 1.5×10^{-2}	3.0	1.1531
1.5×10^{-2} to 2.4×10^{-2}	3.11	0.5912
2.4×10^{-2} to 8.3×10^{-2}	2.6	1.5535
8.3×10^{-2} to 1.35×10^{-1}	3.7	0.6007
1.35×10^{-1} to 2.1×10^{-1}	2.6	0.4791
2.1×10^{-1} to 4×10^{-1}	1.4	0.7525
4×10^{-1} to 5×10^{-1}	2.0	0.2474
5×10^{-1} to 2.0	2.3	1.1460
2.0 to 4.5	7.8	0.2519
4.5 to ∞	8.2	0.0327
Sum of $\left[\lambda^2/3\xi(1 - \overline{\cos\theta}) \times 10^3\right] \left[\int_{V_1}^{V_2} \frac{G(V)}{V} dV\right]$		54.522